

Hybrid Classical-Quantum Models for Charge Transport in Graphene with Sharp Potentials

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Abstract

We give a concise account on the derivation of hybrid quantum-classical models for stationary electron transport in graphene, in presence of sharp potential steps or barriers. A quantum region (an asymptotically thin strip around the potential step or barrier) is coupled through the quantum scattering data to a classical region, where electron transport is described in terms of semiclassical kinetic equations. The diffusive limit of the kinetic model is derived by means of the Chapman-Enskog method, which requires the introduction of a boundary layer corrector and the discussion of a system of coupled Milne problems.

1 Introduction

It is well known that electrons in graphene possess a conical dispersion relation and a discrete degree of freedom, the *chirality* (analogue to photon helicity), making them similar to massless relativistic particles [7]. This fact, combined with the presence of sharp potential profiles, leads to remarkable phenomena such as an highly-selective dependence on the incidence angle of the transmission coefficient through a potential barrier [13], or the "flat lens" properties of a potential step [8]. A fully quantum description of the electronic wave function across the sharp potential interfaces is essential in order to capture such phenomena. On the other hand, far from interfaces, i.e. in regions where the potential is smooth, electrons lose their quantum coherence and one can safely (and more conveniently) resort to a semiclassical kinetic, or even diffusive or hydrodynamic, descriptions [2, 6, 14]. Therefore, in order to have an efficient and accurate mathematical model, it would be desirable to combine the two descriptions into a "hybrid" classical-quantum model.

A hybrid kinetic-quantum model for standard particles (i.e. parabolic and scalar, as opposed to conical and chiral) was firstly considered by Ben Abdallah in Ref. [4]. The stationary model was subsequently extended to the time-dependent case in Ref. [5]. The central idea in Ben Abdallah's construction is that a scattering problem is solved in the quantum region, that is a thin strip around the potential step or barrier, and the resulting scattering states

(incident/reflected/transmitted waves) are identified with inflow/outflow particles in/from the classical region. This leads to a hybrid model where *transmission conditions*, of quantum origin, are imposed to classical kinetic equations. The diffusive limit of Ben Abdallah's model was considered by Degond and El Ayyadi in Ref. [9], where it is shown that *diffusive transmission conditions*, relating the left and right densities across the quantum strip, can be found at first order in the Chapman-Enskog expansion, provided that a suitable boundary layer corrector is introduced (see also Refs. [1, 10]) The quantum information is concentrated into a single constant, the *extrapolation coefficient*, appearing in the diffusive transmission conditions.

In the present work, we first extend the construction of Ref. [4] to the case of electrons in graphene, obtaining a stationary, hybrid kinetic-quantum model represented by semiclassical transport equations coupled by quantum transmission conditions. Then, following Ref. [9], we take the diffusive limit of the quantum-kinetic model, by introducing a suitable boundary layer corrector and applying the Chapman-Enskog procedure. Here, however, because of the chirality degree of freedom, the construction of the boundary corrector leads to the discussion of a system of four (instead of one) half-space, half-range Milne problems. Moreover, the presence of an unbounded negative energy cone forces us to describe negative-energy electrons in terms of holes, which requires the use of Fermi-Dirac statistics. The Fermi-Dirac distributions are eventually approximated by means of suitable Maxwell-Boltzmann distributions. In this way, a stationary, hybrid diffusive-quantum model is obtained which is given by two semiclassical drift-diffusion equations coupled by diffusive transmission conditions, expressed as a system of constraints relating the left/right-electron/hole densities across the quantum strip. The quantum information is therefore concentrated into four constants, namely the asymptotic densities resulting from the solution of the Milne system and appearing in the diffusive transmission conditions as a first-order approximation of the equilibrium diffusive transmission conditions.

The present paper is intended to give a concise presentation of results that will be published separately in a more extended form, and is organized as follows. In Section 2 we briefly review the quantum description of electron dynamics in graphene and its semiclassical limit. Section 3 is devoted to the hybrid kinetic-quantum model. In Section 4 we introduce an electron/hole kinetic description. Section 5 is devoted to the diffusive limit of the kinetic-quantum model and, in particular, to the derivation of the diffusive transmission conditions. Finally, in Section 6, we draw our conclusions by proposing a hybrid diffusive-quantum model that summarises the results of the previous sections.

2 Quantum and semiclassical mechanics of electrons in graphene

Graphene is a 2-dimensional crystal and, therefore, we shall use 2-dimensional position $\mathbf{x} = (x, y)$ and pseudomomentum $\mathbf{p} = (p_x, p_y)$ variables.

The stationary Schrödinger equation for an electron in a graphene sheet, subject to an

electric potential, reads as follows

$$\begin{pmatrix} V/c & P_x - iP_y \\ P_x + iP_y & V/c \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \frac{E}{c} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad (1)$$

where $\mathbf{P} = (P_x, P_y) = -i\hbar\nabla$ is the pseudomomentum operator, $c \approx 10^6$ m/s is the Fermi velocity, $V = V(\mathbf{x})$ is the potential energy and E is the energy eigenvalue. From the spinorial form of the wave function it is apparent that the electron possesses a discrete degree of freedom. This is the so-called *chirality*, which is ultimately related to the presence of two carbon ions in each fundamental cell of the crystal lattice [15], and is represented by the operator

$$\frac{1}{|\mathbf{P}|} \begin{pmatrix} 0 & P_x - iP_y \\ P_x + iP_y & 0 \end{pmatrix},$$

possessing the two eigenvalues $s = 1$ and $s = -1$.

In the semiclassical limit the wave function collapses into states of defined chirality (hereafter labeled by a subscript $s = \pm 1$), and the dynamics is described by the Hamiltonian system

$$\begin{cases} \dot{\mathbf{x}} = \nabla_{\mathbf{p}} E_s(\mathbf{p}), \\ \dot{\mathbf{p}} = -\nabla_{\mathbf{x}} V(\mathbf{x}). \end{cases} \quad (2)$$

We recognize here the main semiclassical quantities associated to electron dynamics in graphene, namely the two energy bands (Dirac cones)

$$E_s(\mathbf{p}) = sc|\mathbf{p}| \quad (3)$$

and the corresponding velocities

$$\mathbf{v}_s = \nabla_{\mathbf{p}} E_s = \frac{sc\mathbf{p}}{|\mathbf{p}|}. \quad (4)$$

From a semiclassical point of view, it is apparent that electrons in graphene move with constant speed c and the direction of motion is either parallel to pseudomomentum, for electrons with positive chirality, or anti-parallel, for electrons with negative chirality. We also remark that the chirality index $s = \pm 1$ (or simply $s = \pm$) can be equally well interpreted as labeling the positive/negative energy cones.

3 Hybrid kinetic-quantum model

For the sake of simplicity, we make the following assumptions on the electric potential:

1. V depends only on the variable x , i.e. $V = V(x)$ (which implies that p_y is conserved);
2. $V(x) \rightarrow 0$ on the left and $V(x) \rightarrow \delta V$ on the right of a “quantum strip”, around $x = 0$, having vanishing width on a macroscopic length scale.

For such potential, the stationary Schrödinger equation (1) has the character of a scattering problem. It is not difficult to see that the scattering states outside the quantum strip are superpositions of waves with defined pseudomomentum \mathbf{p} and chirality s (indeed, this is the feature that makes it possible to interface the quantum scattering solutions with the semiclassical kinetic equations). Moreover, if the left wave (i.e. at $x < 0$) is characterised by (\mathbf{p}, s) and the right wave (i.e. at $x > 0$) is characterised by (\mathbf{p}', s') (recall, however, that p_y is conserved, so that we always have $p_y = p'_y$), then the parameters p_x, s, p'_x, s' are related by the conservation of energy

$$sc|\mathbf{p}| = s'c|\mathbf{p}'| + \delta V, \quad (5)$$

that is

$$s\sqrt{p_x^2 + p_y^2} = s'\sqrt{(p'_x)^2 + p_y^2} + \frac{\delta V}{c}.$$

Solving the scattering problem (1) provides us with the scattering data, i.e. the transmission and reflection coefficients $T_s^i(\mathbf{p})$ and $R_s^i(\mathbf{p})$. Here and in the following, the upper index i indicates the side with respect to $x = 0$. Namely, $i = 1$ refers to the left-hand side ($x < 0$) and $i = 2$ refers to the right-hand side ($x > 0$). For example, $T_s^1(\mathbf{p})$ is the transmission coefficient for an incident wave from the left with energy $E = sc|\mathbf{p}|$, and $T_{s'}^2(\mathbf{p}')$ is the transmission coefficient for an incident wave from the right with energy $E = s'c|\mathbf{p}'| + \delta V$. The transmission and reflection coefficients satisfy the following properties:

1. $T_s^i(\mathbf{p}) \geq$ and $R_s^i(\mathbf{p}) \geq 0$, with $T_s^i(\mathbf{p}) + R_s^i(\mathbf{p}) = 1$ (conservation);
2. $T_s^1(\mathbf{p}) = T_{s'}^2(\mathbf{p}')$, whenever (\mathbf{p}, s) and (\mathbf{p}', s') are related by (5) (reciprocity).

It is worth to remark that the scattering data are known in explicit form in some cases of importance for applications [8, 13].

The quantum part of the model is represented by the scattering problem and the correspondent scattering data. The semiclassical kinetic part of the model is expressed in terms of semiclassical Wigner functions $w_s(\mathbf{x}, \mathbf{p})$, which can be interpreted as phase-space distributions of electrons with positive ($s = +$) and negative ($s = -$) chirality/energy [2, 3]. They satisfy the semiclassical, stationary, transport equation

$$(\mathbf{v}_s \cdot \nabla_{\mathbf{x}} - \nabla_{\mathbf{x}} U \cdot \nabla_{\mathbf{p}}) w_s = \mathcal{C}_s(w_s), \quad (6)$$

which is assumed to hold in the two classical regions, $x > 0$ and $x < 0$. Here, \mathbf{v}_s is the semiclassical velocity (4), \mathcal{C}_s is suitable collisional term and U is an additional smooth potential (we recall that sharp potential V is constant in each classical region).

Let us denote by w_s^i , $i = 1, 2$, the boundary values of w_s , from the left and from the right, at $x = 0$, namely

$$w_s^1(y, \mathbf{p}) = \lim_{x \rightarrow 0^-} w_s(\mathbf{x}, \mathbf{p}), \quad w_s^2(y, \mathbf{p}) = \lim_{x \rightarrow 0^+} w_s(\mathbf{x}, \mathbf{p}).$$

Following the ideas of Ref. [4], we introduce a kinetic-quantum coupling in terms of the following *transmission conditions* (TC):

$$\begin{cases} w_s^1(p_x) = R_s^1(-p_x)w_s^1(-p_x) + T_{s'}^2(p'_x)w_{s'}^2(p'_x), & sp_x, s'p'_x < 0, \\ w_{s'}^2(p'_x) = R_{s'}^2(-p'_x)w_{s'}^2(-p'_x) + T_s^1(p_x)w_s^1(p_x), & s'p'_x, sp_x > 0, \end{cases} \quad (7)$$

where only the relevant variable p_x has been explicitly indicated, and we recall that (p_x, s) and (p'_x, s') are determined each other by (5) (together with the indication of the sign of p_x). The meaning of Eq. (7) is clear: at each side of the quantum strip, the inflow into the classical region is given in part by the reflected outflow from the same side and in part by the transmitted outflow from the opposite side. The fact that the products sp_x and $s'p'_x$ (and not p_x and p'_x alone) determine the outflow or the inflow direction is due to the fact that, as already mentioned, the actual direction of the electron motion is $s\mathbf{p}/|\mathbf{p}|$.

4 Electrons and holes

In order to obtain the diffusive limit of the kinetic-quantum model given by Eqs. (6) and (7), we assume that collisions make the electronic population relax system towards two independent local equilibrium states of defined chirality, parametrized by the density (an assumption which is strictly related to the Maximum Entropy Principle (MEP) [2, 3, 6]). Accordingly, the collisional term in Eq. (6) is assumed to be of BGK type:

$$\mathcal{C}_s(w_s) = \frac{w_s^{\text{eq}} - w_s}{\tau}, \quad (8)$$

where

$$w_s^{\text{eq}} = \frac{1}{e^{s(\beta c|\mathbf{p}| - A_s)} + 1} \quad (9)$$

is a Fermi-Dirac (F-D) distribution, where $\beta = 1/k_B T$, k_B is the Boltzmann constant, T is the temperature and the sign of the chemical potentials A_s has been chosen for later convenience. The MEP requires to impose the constraint that w_s^{eq} and w_s have the same spatial density n_s . By introducing a bracket notation for the normalised integrals [2] with respect to \mathbf{p} ,

$$\langle \cdot \rangle = \frac{1}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} \cdot d\mathbf{p}, \quad (10)$$

we express such constraint as

$$\langle w_s^{\text{eq}} \rangle = n_s. \quad (11)$$

However, since the lower energy cone is unbounded from below (see Eq. (3)), w_-^{eq} cannot have finite moments, and Eq. (11) does not make sense for $s = -1$. In order to fix this, we have to describe negative-energy/chirality electrons in term of electron vacancies (*holes*). Let us therefore introduce the distributions f_+ (electrons) and f_- (holes) defined by

$$f_+(\mathbf{x}, \mathbf{p}) = w_+(\mathbf{x}, \mathbf{p}), \quad f_-(\mathbf{x}, \mathbf{p}) = 1 - w_-(\mathbf{x}, -\mathbf{p}). \quad (12)$$

Note that the definition of f_- contains a change in the sign of \mathbf{p} , so that holes move parallel to \mathbf{p} . By applying the transformation (12) to Eq. (6) (with \mathcal{C}_s given by (8)), we obtain

$$\left(\frac{c\mathbf{p}}{|\mathbf{p}|} \cdot \nabla_{\mathbf{x}} - s \nabla_{\mathbf{x}} U \cdot \nabla_{\mathbf{p}} \right) f_s = \frac{f_s^{\text{eq}} - f_s}{\tau} \quad (13)$$

where

$$f_s^{\text{eq}} = \frac{1}{e^{\beta c|\mathbf{p}| - A_s} + 1} \quad (14)$$

are now F-D distributions both with *positive* energies, so that we can safely impose the constraint

$$\langle f_s^{\text{eq}} \rangle = n_s. \quad (15)$$

This fixes the chemical potentials A_s as functions of the densities n_s as follows [2]:

$$\phi_2(A_s) = \frac{n_s}{n_0}, \quad (16)$$

where

$$\phi_k(z) = \frac{1}{\Gamma(k)} \int_0^\infty \frac{t^{k-1}}{e^{t-z} + 1} dt, \quad (17)$$

is the Fermi integral of order $k > 0$, and

$$n_0 = \frac{2\pi}{(2\pi\hbar c\beta)^2} = \frac{(k_B T)^2}{2\pi\hbar^2 c^2}. \quad (18)$$

For large T , the relation (16) is well approximated by

$$e^{A_s} \approx \frac{n_s}{n_0}, \quad (19)$$

which corresponds to approximating the F-D distribution (14) with the Maxwell-Boltzmann (M-B) distribution

$$f_s^{\text{eq}} \approx n_s M, \quad M(\mathbf{p}) = \frac{1}{n_0} e^{-\beta c|\mathbf{p}|}, \quad (20)$$

with $\langle M \rangle = 1$.

Remark 4.1 *It is important to remark that the TC (7) hold for w_s 's and, then, when applying the TC to the f_s 's, one has to perform the transformation (12) before.*

By using the conservation and reciprocity properties of the reflection and transmission coefficients, it is possible to prove the following

Proposition 4.2 (Current conservation) *The TC (7) conserve the total current across the quantum strip, i.e.*

$$\mathbf{J}_+^1 + \mathbf{J}_-^1 = \mathbf{J}_+^2 + \mathbf{J}_-^2, \quad (21)$$

where

$$\mathbf{J}_s = \left\langle \frac{c\mathbf{p}}{|\mathbf{p}|} f_s \right\rangle \quad (22)$$

and, in accordance with the convention introduced in the previous section, \mathbf{J}_s^1 and \mathbf{J}_s^2 denote the left and right limits of \mathbf{J}_s at $x = 0$.

5 Diffusive limit

Following the Chapman-Enskog (C-E) procedure, the diffusion asymptotics is obtained from the expansion of the unknown functions f_s in powers of the relaxation time τ , to be considered as a small parameter in Eq. (13):

$$f_s = f_s^{(0)} + \tau f_s^{(1)} + o(\tau). \quad (23)$$

Substituting (23) into (13) and equating the coefficients of equal powers of τ at the two sides yields

$$f_s^{(0)} = f_s^{\text{eq}}, \quad f_s^{(1)} = - (f_s^{\text{eq}})^2 e^{\beta c |\mathbf{p}| - A_s} \frac{c \mathbf{p}}{|\mathbf{p}|} \cdot (\nabla A_s + s \beta \nabla U). \quad (24)$$

It will be convenient to rewrite $f_s^{(1)}$ as follows:

$$f_s^{(1)} = \mathbf{L}_s \cdot \mathbf{j}_s, \quad (25)$$

where

$$\mathbf{L}_s = \frac{2 (f_s^{\text{eq}})^2 e^{\beta c |\mathbf{p}| - A_s}}{c n_0 \phi_1(A_s)} \frac{\mathbf{p}}{|\mathbf{p}|} \quad (26)$$

and

$$\mathbf{j}_s = -\frac{c^2}{2} n_0 \phi_1(A_s) [\nabla A_s + s \beta \nabla U] = -\frac{c^2}{2} [\nabla n_s + s \beta n_0 \phi_1(A_s) \nabla U]. \quad (27)$$

From (22), after some algebra, we obtain that the current is given at order τ by

$$\mathbf{J}_s = \langle \frac{c \mathbf{p}}{|\mathbf{p}|} f_s^{\text{eq}} \rangle + \tau \langle \frac{c \mathbf{p}}{|\mathbf{p}|} f_s^{(1)} \rangle + o(\tau) = \tau \mathbf{j}_s + o(\tau). \quad (28)$$

In the M-B approximation, the preceding expressions become $f_s^{(0)} = n_s M$ and $f_s^{(1)} = \mathbf{L} \cdot \mathbf{j}_s$, with

$$\mathbf{j}_s = -\frac{c^2}{2} [\nabla n_s + s \beta n_s \nabla U], \quad \mathbf{L} = \frac{2M}{c} \frac{\mathbf{p}}{|\mathbf{p}|}, \quad (29)$$

Taking $\langle \cdot \rangle$ of both sides of Eq. (13), and using (15), yields $\text{div } \mathbf{j}_s = 0$ and then, from Eq. (28), we obtain that the stationary drift-diffusion equations

$$\frac{\tau c^2}{2} \text{div} [\nabla n_s + s \beta n_0 \phi_1(A_s) \nabla U] = 0, \quad (30)$$

or its M-B approximation

$$\frac{\tau c^2}{2} \text{div} [\nabla n_s + s \beta n_s \nabla U] = 0, \quad (31)$$

hold up to terms $o(\tau)$. The multiplicative constant is clearly irrelevant here but becomes important in the time-dependent framework [2].

5.1 Diffusive transmission conditions at leading order

In order to expand the transmission conditions it is convenient to introduce the transformation $f_s \mapsto \tilde{f}_s$ defined as follows:

$$\tilde{f}_+(\mathbf{x}, \mathbf{p}) = f_+(\mathbf{x}, \mathbf{p}), \quad \tilde{f}_-(\mathbf{x}, \mathbf{p}) = 1 - f_-(\mathbf{x}, \mathbf{p}), \quad (32)$$

that is, recalling (12),

$$\tilde{f}_s(\mathbf{x}, \mathbf{p}) = w_s(\mathbf{x}, s\mathbf{p}) \quad (33)$$

In this way, by also exploiting the conservation and reciprocity properties of $T_s^i(\mathbf{p})$ and $R_s^i(\mathbf{p})$, the TC (7) can be written as follows:

$$\begin{cases} \tilde{f}_s^1(-p_x) - \tilde{f}_s^1(p_x) + T_s^1(p_x) [\tilde{f}_s^1(p_x) - \tilde{f}_{s'}^2(-p'_x)] = 0, & p_x, p'_x > 0, \\ \tilde{f}_{s'}^2(p'_x) - \tilde{f}_{s'}^2(-p'_x) + T_{s'}^2(p'_x) [\tilde{f}_{s'}^2(-p'_x) - \tilde{f}_s^1(p_x)] = 0, & p'_x, p_x > 0, \end{cases} \quad (34)$$

where now p_x and p'_x are always positive and we recall that \mathbf{p} and \mathbf{p}' are linked by the conservation of energy (5). We also used the fact that $T_{s'}^2(-p'_x) = T_{s'}^2(p'_x)$, because the scattering coefficients only depend on energy. Equation (34) will be shortly written as

$$\mathcal{B}(\tilde{f}) = 0, \quad (35)$$

where $\tilde{f} = (\tilde{f}_+^1, \tilde{f}_-^1, \tilde{f}_+^2, \tilde{f}_-^2)$ and we remark that \mathcal{B} is linear in \tilde{f} .

It is easily seen that the first two terms in the C-E expansion $\tilde{f}_s = \tilde{f}_s^{(0)} + \tau \tilde{f}_s^{(1)} + o(\tau)$ of \tilde{f}_s are given by

$$\tilde{f}_s^{(0)} = w_s^{\text{eq}}, \quad \tilde{f}_s^{(1)} = s f_s^{(1)}, \quad (36)$$

where we recall that $f^{(1)}$ is given by (24). Then, at leading order in Eq. (35), we have to impose

$$\mathcal{B}(w^{\text{eq}}) = 0, \quad (37)$$

which implies

$$\frac{1}{e^{\beta cs|\mathbf{p}| - sA_s^1} + 1} = \frac{1}{e^{\beta cs'|\mathbf{p}'| - s'A_{s'}^2} + 1},$$

that is, using (5),

$$\frac{1}{e^{\beta cs|\mathbf{p}| - sA_s^1} + 1} = \frac{1}{e^{\beta cs|\mathbf{p}| - s'A_{s'}^2 - \beta \delta V} + 1}. \quad (38)$$

We obtain therefore a condition relating left and right chemical potentials,

$$sA_s^1 = s'A_{s'}^2 + \beta \delta V, \quad (39)$$

which holds for s and s' that can be connected by the conservation of energy (5). Assuming, without loss of generality, $\delta V \geq 0$ we have three possibilities,

$$(s, s') = (+, +), \quad (s, s') = (+, -), \quad (s, s') = (-, -),$$

if $\delta V > 0$, or just two,

$$(s, s') = (+, +), \quad (s, s') = (-, -),$$

if $\delta V = 0$. In the M-B approximation Eq. (19) holds and we obtain the following explicit relation between left and right densities in the two cones:

$$\begin{aligned} n_+^1 &= e^{\beta\delta V} n_+^2, \\ n_-^1 &= e^{-\beta\delta V} n_-^2, \\ n_+^1 n_-^2 &= e^{\beta\delta V} (n_0)^2. \end{aligned} \tag{40}$$

Remark 5.1 *According to the above discussion, the third equation is present if and only if $\delta V > 0$. Note that, in this case, left electrons and right holes (and conversely) are connected by a mass-action law.*

5.2 Diffusive transmission conditions at order τ

Coming to the first order, we should impose $\mathcal{B}(sf^{(1)}) = 0$. However, it turns out that $\mathcal{B}(sf^{(1)})$ is in general different from zero, which means that it is impossible to fit the TC at order τ in the C-E expansion. This difficulty is not new in similar situations considered in literature, and is overcome by introducing a suitable boundary layer corrector [9, 10].

To this aim, let us magnify the layer by stretching the x variable by a factor proportional to $1/\tau$, i.e. by introducing the layer variable $\xi = x/\tau$. In terms of ξ , when $\tau \rightarrow 0$, the transport equation (13) reduces to

$$c\mu \frac{\partial f_s}{\partial \xi} + f_s = f_s^{\text{eq}}, \tag{41}$$

where

$$\mu = \frac{p_x}{|\mathbf{p}|} \tag{42}$$

is the cosine of the incidence angle. Then we look for four functions, θ_s^i , $i = 1, 2$, $s = \pm 1$, that solve

$$c\mu \frac{\partial \theta_s^1}{\partial \xi} + \theta_s^1 = \theta_s^{1,\text{eq}}, \quad \xi < 0, \quad \mathbf{p} \in \mathbb{R}^2, \quad s = \pm 1, \tag{43a}$$

$$c\mu \frac{\partial \theta_s^2}{\partial \xi} + \theta_s^2 = \theta_s^{2,\text{eq}}, \quad \xi > 0, \quad \mathbf{p} \in \mathbb{R}^2, \quad s = \pm 1 \tag{43b}$$

$$\mathcal{B}(\tilde{\theta}) = \mathcal{B}(h), \quad \xi = 0, \quad \mathbf{p} \in \mathbb{R}^2, \tag{43c}$$

where $\theta_s^{i,\text{eq}}$ are F-D distributions such that

$$\langle \theta_s^{i,\text{eq}} \rangle = \langle \theta_s^i \rangle. \tag{44}$$

and we have put

$$h_s = sf_s^{(1)} = s \mathbf{L}_s \cdot \mathbf{j}_s \tag{45}$$

Equation (43) is a system of four half-space, half-range Milne problems [11] coupled by the non-homogeneous transmission condition (43c). By using classical results on Milne problems [1] it is possible to prove the following

Theorem 5.2 (Asymptotic solution to the coupled Milne problems) *Four constants $A_s^{i,\infty}$ exist such that*

$$\theta_s^i \rightarrow \theta_s^{i,\infty} := \frac{1}{e^{\beta c|\mathbf{p}| - A_s^{i,\infty}} + 1}, \quad \text{as } \xi \rightarrow (-1)^i \infty, \quad (46)$$

and the convergence is exponentially fast.

We can now modify the C-E ansatz (23) by inserting a layer corrector of order τ :

$$f_s = f_s^{\text{eq}} + \tau f_s^{(1)} - \tau(\theta_s - \theta_s^\infty) + o(\tau), \quad (47)$$

where

$$\theta_s = \begin{cases} \theta_s^1 & x < 0, \\ \theta_s^2 & x > 0, \end{cases} \quad \theta_s^\infty = \begin{cases} \theta_s^{1,\infty} & x < 0, \\ \theta_s^{2,\infty} & x > 0, \end{cases} \quad (48)$$

and where we have substituted back the original variable x in the functions θ_s^i and $\theta_s^{i,\infty}$. Then, according to Theorem 5.2, $\tau(\theta_s - \theta_s^\infty)$ decays as $\tau \exp(-C|x|/\tau)$, for some constant $C > 0$. In this way the drift-diffusion equation (30) is left unchanged in the bulk classical regions and the corrector only affects the TC (35).

In order to evaluate the TC (35), we note that the C-E expansion of \tilde{f} reads as follows:

$$\tilde{f}_s = w_s^{\text{eq}} + \tau h - \tau(\tilde{\theta}_s - \tilde{\theta}_s^\infty) + o(\tau), \quad (49)$$

where we used (45) and the identity $s(\theta_s - \theta_s^\infty) = \tilde{\theta}_s - \tilde{\theta}_s^\infty$. Then, the evaluation of $\mathcal{B}(\tilde{f})$ yields

$$\mathcal{B}(\tilde{f}) = \mathcal{B}(w^{\text{eq}}) + \tau \mathcal{B}(h) - \tau \mathcal{B}(\tilde{\theta}) + \tau \mathcal{B}(\tilde{\theta}^\infty) + o(\tau) = \mathcal{B}(w^{\text{eq}}) + \tau \mathcal{B}(\tilde{\theta}^\infty) + o(\tau),$$

where (43c) was used. Therefore, the approximation at order τ of the TC (35) is

$$\mathcal{B}(w^{\text{eq}} + \tau \tilde{\theta}^\infty) = 0, \quad (50)$$

which yields

$$\frac{1}{e^{\beta c s |\mathbf{p}| - s A_s^1} + 1} - \frac{1}{e^{\beta c s' |\mathbf{p}'| - s' A_{s'}^2} + 1} = \frac{\tau}{e^{\beta c s' |\mathbf{p}'| - s' A_{s'}^{2,\infty}} + 1} - \frac{\tau}{e^{\beta c s |\mathbf{p}| - s A_s^{1,\infty}} + 1},$$

that is

$$\frac{1}{e^{\beta c s |\mathbf{p}| - s A_s^1} + 1} - \frac{1}{e^{\beta c s |\mathbf{p}| - s' A_{s'}^2 - \beta \delta V} + 1} = \frac{\tau}{e^{\beta c s |\mathbf{p}| - s' A_{s'}^{2,\infty} - \beta \delta V} + 1} - \frac{\tau}{e^{\beta c s |\mathbf{p}| - s A_s^{1,\infty}} + 1}. \quad (51)$$

Condition (51) should be satisfied for all s , s' and \mathbf{p} such that the conservation of energy (5) holds for some \mathbf{p}' . This is in general a too demanding condition. However, it can be satisfied in the M-B approximation (20), which leads to

$$e^{s A_s^1} - e^{\beta \delta V} e^{s' A_{s'}^2} = \tau \left(e^{\beta \delta V} e^{s' A_{s'}^{2,\infty}} - e^{s A_s^{1,\infty}} \right)$$

or, using (19),

$$\left(\frac{n_s^1}{n_0}\right)^s - e^{\beta\delta V} \left(\frac{n_{s'}^2}{n_0}\right)^{s'} = \tau \left[e^{\beta\delta V} \left(\frac{n_{s'}^{2,\infty}}{n_0}\right)^{s'} - \left(\frac{n_s^{1,\infty}}{n_0}\right)^s \right]. \quad (52)$$

If $\delta V > 0$ the last equation gives three first-order conditions

$$\begin{aligned} n_+^1 - e^{\beta\delta V} n_+^2 &= \tau \left(e^{\beta\delta V} n_+^{2,\infty} - n_+^{1,\infty} \right), \\ n_-^1 - e^{-\beta\delta V} n_-^2 &= \tau \left(e^{-\beta\delta V} n_-^{2,\infty} - n_-^{1,\infty} \right), \\ \frac{n_+^1}{n_0} - e^{\beta\delta V} \frac{n_0}{n_-^2} &= \tau \left(e^{\beta\delta V} \frac{n_0}{n_-^{2,\infty}} - \frac{n_+^{1,\infty}}{n_0} \right), \end{aligned} \quad (53)$$

while for $\delta V = 0$ the third condition disappears. Note that (53) represents a (quantum) correction of order τ to the equilibrium conditions (40).

Remark 5.3 *The M-B approximation of (51) needs to be explained in more details. Focusing on the right-hand side (the left-hand side is treated in the same way), we have made the following approximations:*

$$\frac{1}{e^{\beta c|\mathbf{p}| - A_+^1} + 1} - \frac{1}{e^{\beta c|\mathbf{p}| - A_+^2 - \beta\delta V} + 1} \approx e^{-\beta c|\mathbf{p}| + A_+^1} - e^{-\beta c|\mathbf{p}| + A_+^2 + \beta\delta V},$$

when $s = s' = +$,

$$\begin{aligned} \frac{1}{e^{-\beta c|\mathbf{p}| + A_-^1} + 1} - \frac{1}{e^{-\beta c|\mathbf{p}| + A_-^2 - \beta\delta V} + 1} &= -\frac{1}{e^{\beta c|\mathbf{p}| - A_-^1} + 1} + \frac{1}{e^{\beta c|\mathbf{p}| - A_-^2 + \beta\delta V} + 1} \\ &\approx -e^{-\beta c|\mathbf{p}| + A_-^1} + e^{-\beta c|\mathbf{p}| + A_-^2 - \beta\delta V}, \end{aligned}$$

when $s = s' = -$, and

$$\frac{1}{e^{\beta c|\mathbf{p}| - A_+^1} + 1} - \frac{1}{e^{\beta c|\mathbf{p}| + A_-^2 - \beta\delta V} + 1} \approx e^{-\beta c|\mathbf{p}| + A_+^1} - e^{-\beta c|\mathbf{p}| - A_-^2 + \beta\delta V},$$

when $s = +$ and $s' = -$. Note, in particular, that left electrons in the lower cone are treated as holes (and their distribution is approximated by $e^{-\beta c|\mathbf{p}'| + A_-^2}$) in the $(-, -)$ zone, while they are treated as negative-energy electrons (and their distribution is approximated by $e^{\beta c|\mathbf{p}'| - A_-^2}$) in the $(+, -)$ zone (if present). These approximations are compatible with a situation in which

$$A_+^1 \approx A_-^1 \approx 0, \quad A_+^2 \approx -\beta\delta V, \quad A_-^2 \approx \beta\delta V.$$

6 Conclusions

Let an hypothetical graphene device be represented by the rectangle $(x, y) \in (-L, L) \times (-l, l)$, where the quantum step/barrier is concentrated in $x = 0$ (on a macroscopic scale), and the two classical regions are

$$\Omega^1 = (-L, 0) \times (-l, l), \quad \text{and} \quad \Omega^2 = (0, L) \times (-l, l).$$

To be consistent with the approximations introduced in Section 5.2, we shall assume to work in the M-B approximation. Then, in Ω^1 and Ω^2 the stationary drift-diffusion equation (31) is assumed to hold. At the external boundary of the device the standard conditions can be imposed, e.g. non homogeneous Dirichlet conditions at $x = -L$ and $x = L$ (representing ohmic contacts) and homogeneous Neumann conditions at $y = -l$ and $y = l$ (representing insulation). At the quantum-classical interface, $x = 0$, the DTC (53) are imposed.

If $\delta V > 0$, the DTC is a rank-3 condition and we still need a further condition, which is given by the total current conservation (21) projected along the x axis (recall that the drift-diffusion current \mathbf{J}_s coincides with the total current at order τ , thanks to Eq. (28)).

In summary, the hybrid diffusive-quantum model we propose is the following:

$$\left. \begin{aligned} \operatorname{div} \mathbf{J}_s &= 0 \\ \mathbf{J}_s &= -\nabla n_s - s\beta n_s \nabla U \end{aligned} \right\}, \quad \text{in the semiclassical regions } \Omega^1 \cup \Omega^2,$$

$$n_s = n_s^{\pm L}, \quad \text{at the Ohmic boundary } x = \pm L,$$

$$\mathbf{e}_y \cdot \mathbf{J}_s = 0, \quad \text{at the insulating boundary } y = \pm l,$$

$$\left. \begin{aligned} n_+^1 - e^{\beta\delta V} n_+^2 &= \tau \left(e^{\beta\delta V} n_+^{2,\infty} - n_+^{1,\infty} \right) \\ n_-^1 - e^{-\beta\delta V} n_-^2 &= \tau \left(e^{-\beta\delta V} n_-^{2,\infty} - n_-^{1,\infty} \right) \\ \frac{n_+^1}{n_0} - e^{\beta\delta V} \frac{n_0}{n_-^2} &= \tau \left(e^{\beta\delta V} \frac{n_0}{n_-^{2,\infty}} - \frac{n_+^{1,\infty}}{n_0} \right) \\ \mathbf{e}_x \cdot (\mathbf{J}_+^1 + \mathbf{J}_-^1 - \mathbf{J}_+^2 - \mathbf{J}_-^2) &= 0 \end{aligned} \right\}, \quad \text{across the quantum interface } x = 0, \quad (54)$$

where $n_s^{\pm L}$ are the given densities of electrons and holes at the contacts, and \mathbf{e}_x , \mathbf{e}_y are the directions of the x and y axes.

If $\delta V = 0$, then the third DCT equation disappear and we are left with a rank-2 condition. However, in this case, the current conservation holds *separately* for electrons and holes and we gain one more condition on current. If $\delta V = 0$, therefore the conditions across the interface are substituted by

$$\left. \begin{aligned} n_+^1 - e^{\beta\delta V} n_+^2 &= \tau \left(e^{\beta\delta V} n_+^{2,\infty} - n_+^{1,\infty} \right) \\ n_-^1 - e^{-\beta\delta V} n_-^2 &= \tau \left(e^{-\beta\delta V} n_-^{2,\infty} - n_-^{1,\infty} \right) \\ \mathbf{e}_x \cdot (\mathbf{J}_+^1 - \mathbf{J}_+^2) &= 0 \\ \mathbf{e}_x \cdot (\mathbf{J}_-^1 - \mathbf{J}_-^2) &= 0 \end{aligned} \right\}, \quad (55)$$

and the problems for electrons and holes become completely decoupled.

The densities $n_s^{i,\infty}$ are obtained by solving the system of Milne equations (43). This means that $n_s^{i,\infty}$ depends on \mathbf{J}_s and, therefore, the DTC couple the four (left/right, electrons/holes) drift-diffusion equations in (54). We also remark that the functions $n_s^{i,\infty}$ embody the quantum part of the model, represented by the scattering problem (1).

Of course, solving the coupled Milne equations (43) is in general an hard numerical task, and the advantage of the diffusive-quantum model (54), with respect to the kinetic-quantum one, is far from being evident. It is therefore necessary to reduce the complexity of problem (43), which can be done by means of a Maxwellian approximation of the solution to the albedo problem associated to Eq. (41) [9], or by means of the iterative procedure proposed by Golse and Klar [12].

We finally remark that, in the present formulation, the quantum part of the problem is independent of the semiclassical one, to the extent that the scattering problem (1) is solved, self-consistently and once for all, in order to get the scattering data. However, a more complicate nonlinear coupling can be introduced by assuming that the quantum potential V depends in part on the densities n_s through a Poisson equation [4, 9].

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